

## **Reinforcing chalcogen bonds through alkaline-earth bonds**

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G4 calculations show that the strength of chalcogen interactions is dramatically enhanced by the presence of alkaline-earth bonds. Cooperativity between these two kinds of non-covalent interactions is studied exploring different complexes between chalcogen derivatives, alkaline-earth derivatives and N-bases. In terms of binding energies, chalcogen bonds in ternary complexes can be enhanced by one order of magnitude with respect to binary complexes. This is due to the interplay of all non-covalent interactions involved: the strong cooperativity between chalcogen and alkaline-earth bonds, and the appearance of secondary non-covalent interactions (hydrogen bonds). These results will be compared to other previous results from our group in cooperativity phenomena.

## **References**

1. C. Martín-Fernández, M. M. Montero-Campillo, I. Alkorta, M. Yáñez, O. Mó, J. Elguero, *Chem Eur J.* **24** (2018), 1971.
2. M. Merced Montero-Campillo, P. Sanz, O. Mó, M. Yáñez, I. Alkorta, J. Elguero, *PhysChemChemPhys* **20** (2018), 2413.